The Scientific Advisory Board of the GM/CA Beam line discussed the reports from the different synchrotron facilities on March 27, 2006 via conference call. Those participating included Lonny Berman, Stephen Burley, Zbyszek Dauter, Thomas Earnest, Shelagh Ferguson-Miller, Peter Kuhn, Charles Edmonds and John Johnson. During the teleconference, two members of the committee, Lonny Berman and Thomas Earnest, recused themselves from the committee discussions pertaining to the activities at the facilities where they may be viewed as having a conflict of interest, NSLS and ALS respectively.

Introduction to the NIGMS supplements initiative

The supplements initiative was proposed in 1998. John Norvell submitted letters to the directors of facilities which hosted macromolecular crystallography programs, to request funding for upgrades at their respective facilities that would serve to enhance user access for macromolecular crystallography.

In response, every facility that upheld a crystallography capability at that time submitted a request. This was a multi-step process, whereby the original solicitation letter to the facility directors was followed by submission of letters of intent by the facility directors, to which John Norvell responded with formal invitations for requests for funding.

The requests were evaluated by NIGMS in early 1999, before the formation of the GM/CA SAB. John Norvell convened an ad-hoc committee to evaluate these requests. Several, but not all, of these requests were funded wholly or in part. Thereafter, John Norvell and Marvin Cassman agreed to convene a new committee, which is the present GM/CA SAB, to commence discussions strictly about forming a new CAT for the APS which would be funded and managed jointly by NIGMS and NCI. The present SAB held its inaugural meeting in June 1999. In 2003, the SAB's charge was expanded, to also provide feedback about the activities at the other synchrotron radiation facilities that were sponsored by the NIGMS supplements initiative.

Discussion of the NSLS program 839K

This is a unique effort in terms of the NIGMS funding in that the beam line was implemented de novo for the purpose of macromolecular crystallography and it is totally supported by this NIGMS funding mechanism (this approach is the same approach taken by NIGMS for its investment at the APS, although the APS investment isn't part of this supplements activity). Therefore, unlike the cases of the supplements-funded activities at the other synchrotron radiation sources (which derive core funding support from elsewhere, the information for which wasn't provided for this evaluation), it is rather straightforward to establish, in the case of the activity at NSLS, the impact of the supplemental support provided by NIGMS. All of the cited productivity described in the report from NSLS stems directly, and only, from the support provided by NIGMS through this activity. There were 180 users of the facility in the last year representing 80 projects. There were 18 PDB submissions and 29 publications that resulted from the work at this beam line. This is the most service-oriented facility with little research

contributions. There are efforts at implementing various developments from other synchrotrons including the Berkeley auto-mounter.

While there was a concern expressed by a subset of the SAB about the relative cost effectiveness of the NIGMS investment at NSLS as compared with the counterpart NIGMS investments at the other facilities, the evaluators were unable to sensibly establish a meaningful comparison because the reports from the other facilities did not describe their levels of core funding support which were supplemented by the NIGMS funding through this activity. As a result it was not possible to establish the relative impact of the supplemental support provided by NIGMS to the other facilities, whereas in the case of the NIGMS investment at NSLS it was easy to establish. A subset of the SAB expressed a concern about the NIGMS investment at NSLS being focused exclusively on a bending magnet beamline program, whereas the NIGMS investments at the other facilities were applied to a mix of bending magnet and (mostly) insertion device beamline programs. Nevertheless, the strategy pursued for the NIGMS investment at NSLS was endorsed by NIGMS at the start of the initiative, in favor of alternative but costlier proposed options that would have involved an insertion device beamline.

Discussion of the future of this supplemental support activity

There were a number of points that were discussed regarding the next evaluation of funding distributed in this initiative. Generally the committee agreed that the diversity of these facilities was a good thing and we do not want one size to fit all. However, there is disappointment in the fact that these funds have not encouraged more cooperation between user facilities to maximize the positive experiences at the different beam lines. There should be mechanisms for more extensive sharing between these facilities and the NIGMS/NCI (GM/CA) sector at APS should be brought under the umbrella of this activity in order to integrate it into the larger GM supported efforts for structure determination. There is too much parallel effort, such as in crystal centering development where this could be done cooperatively.

All members of the committee felt that it was important to have a detailed “other support” page in the next renewal so that it is clear what fraction this funding initiative makes to the total. As mentioned several times already in this report, having an appreciation of such information would facilitate the committee’s evaluations of these activities, for it would help to establish the relative impact of the support provided by NIGMS. The committee will also be looking for evidence of synergy between the different facilities supported by this initiative. Moreover, efforts will be made to distribute these funds (potentially in a way different from its current form) to obtain the maximum productivity users of these facilities. While this is likely to be in a more competitive process, the committee emphasizes that it wants to maintain the existing novelty associated with the facilities.

A more thorough discussion of ways to approach this will be discussed at the GM/CA SAB meeting in Chicago in June. At this meeting, it will be important to understand precisely what role the GM/CA SAB is expected to play in evaluating this worthwhile

initiative. On multiple occasions now, the evaluation team has been asked to conduct a critique of NIGMS-funded operations at CHESS, ALS, NSLS, and SSRL without the possibility of influencing further funding decisions. On its face, this would not appear to be the best use of the GM/CA SAB.